

# Ethanone, 2-ethoxy-1-phenyl-

|                      |                                                                 |
|----------------------|-----------------------------------------------------------------|
| Inchi:               | InChI=1S/C10H12O2/c1-2-12-8-10(11)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3 |
| InchiKey:            | RBMWDBHKRZTOMB-UHFFFAOYSA-N                                     |
| Formula:             | C10H12O2                                                        |
| SMILES:              | CCOCC(=O)c1ccccc1                                               |
| Mol. weight [g/mol]: | 164.20                                                          |
| CAS:                 | 14869-39-7                                                      |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -88.19  | kJ/mol  | Joback Method  |
| hf            | -258.00 | kJ/mol  | Joback Method  |
| hfus          | 18.48   | kJ/mol  | Joback Method  |
| hvap          | 49.29   | kJ/mol  | Joback Method  |
| log10ws       | -2.06   |         | Crippen Method |
| logp          | 1.906   |         | Crippen Method |
| mcvol         | 135.440 | ml/mol  | McGowan Method |
| pc            | 3082.99 | kPa     | Joback Method  |
| tb            | 531.17  | K       | Joback Method  |
| tc            | 743.85  | K       | Joback Method  |
| tf            | 301.04  | K       | Joback Method  |
| vc            | 0.511   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 300.47    | J/mol×K | 531.17          | Joback Method |
| cpg           | 361.01    | J/mol×K | 708.40          | Joback Method |
| cpg           | 350.35    | J/mol×K | 672.95          | Joback Method |
| cpg           | 338.99    | J/mol×K | 637.51          | Joback Method |
| cpg           | 326.90    | J/mol×K | 602.06          | Joback Method |
| cpg           | 314.07    | J/mol×K | 566.62          | Joback Method |
| cpg           | 370.98    | J/mol×K | 743.85          | Joback Method |
| dvisc         | 0.0002164 | Pa×s    | 531.17          | Joback Method |
| dvisc         | 0.0002757 | Pa×s    | 492.81          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003660 | Pa×s | 454.46 | Joback Method |
| dvisc | 0.0005118 | Pa×s | 416.11 | Joback Method |
| dvisc | 0.0007662 | Pa×s | 377.75 | Joback Method |
| dvisc | 0.0012567 | Pa×s | 339.39 | Joback Method |
| dvisc | 0.0023380 | Pa×s | 301.04 | Joback Method |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C14869397&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14869397&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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